Concatenated Control Sequences based on Optimized Dynamic Decoupling

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Two recent developments in quantum control, concatenation and optimization of pulse intervals, are combined to yield a strategy to suppress unwanted couplings in quantum systems to high order. Longitudinal relaxation and transverse dephasing can be suppressed so that systems with a small splitting between their energy levels can be kept isolated from their environment. The required number of pulses grows exponentially with the desired order but is only the square root of the number needed if only concatenation is used. An approximate scheme even brings the number down to polynomial growth. The approach is expected to be useful for quantum information and for high-precision nuclear magnetic resonance.

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If one wants to measure small shifts in local energy levels high-precision nuclear magnetic resonance (NMR) is a powerful means of investigation. In order to reduce the line widths which limit the achievable resolution it is important to isolate the system under study as much as possible from its environment. It is common in NMR to do this by intricate sequences of pulses, see e.g. Ref. 1.

Similarly, one of the big hurdles in the realization of quantum information (QI) is to keep information stored without loss due to decoherence. Besides quantum error correction, see e.g. [2, 3], dynamic decoupling (DD) is one important tool to reduce decoherence [4, 5, 6, 7, 8, 9]. Here, as for NMR, a sequence of pulses is used to achieve an effective Hamiltonian where the quantum bit (qubit) is as much isolated from its environment as possible.

So in both these fascinating areas of physics the design of appropriate pulse sequences is of great relevance.

The fundamental idea is to compensate the effect of a Hamiltonian (or a part of it) by inverting its sign by a π pulse. This is known since long as spin-echo technique [10] which works very nicely for static magnetic fields. Its sequence reads $p_{\rm SE} = f_\tau \, \pi \, f_\tau$. Further improvement is obtained by passing to the combination of two pules in $p_{\rm CPMG} = f_\tau \, \pi \, f_{2\tau} \, \pi \, f_\tau$ [11, 12] which is commonly called CPMG after the first letters of its inventors. The total duration of the cycle is $t = 4\tau$. Here π stands for an ideal, instantaneous π pulse which takes a part of the Hamiltonian to its negative while f_τ stand for the time evolution due to the unchanged Hamiltonian over the interval τ. Both basic cylces are commonly iterated: the iteration of the spin echo leads to $p_{\rm PDD} = f_\tau \, (\pi \, f_\tau)^n$ with $t = (n+1)\tau$ which is often called periodic dynamic decoupling (PDD). The iteration of the CPMG leads to $p_{\rm iCPMG} = (f_\tau \, \pi \, f_\tau)^{2n}$ with $t = 2n\tau$ which is successful in many circumstances, see for instance Refs. 13, 14. It is particularly robust against soft high-energy cutoffs [15, 16].

Recently, two powerful extensions of DD have been proposed. The first is concatenation [8, 17] (CDD). By iterating the concatenation of pulse sequences $p_{n+1} = p_n \, X \, p_n \, Z \, p_n \, X \, p_n \, Z$ with $p_0 = f_\tau$ Khodjasteh and Lidar could show that the interaction between a qubit and its environment can be reduced to order t^{n+1}. Hereby X stands for a π pulse about σ_X, the Pauli matrix of the qubit in x-direction, and Z stands for a π pulse about σ_Z. The caveat of this approach is that the number of necessary pulses grows exponentially with a high power $\propto 4^n$ with the concatenation level n, thus with the power in t. Hence the implementation of a CDD sequence for a given order can be technically very demanding.

The second extension is the optimization of the intervals between the pulses. They need not be chosen equidistant and this additional degree of freedom can be exploited for optimization [9] leading to the UDD sequence. In a dephasing model where bosons are coupled linearly to the qubit (spin-boson model) the author showed that the instants $\tilde{\delta}_j$ ($j \in \{1, 2, \ldots n\}$) for π pulses are optimum if

$$\tilde{\delta}_j = t \sin^2(\pi j/(2(n+1))). \qquad (1)$$

Based on the observation that this formula does not depend on any details of the system and on the knowledge that most degrees of freedom behave at high temperatures like gaussian fluctuations the author concluded this sequence is not specific to the spin-boson model. The main advantage of $p_{\rm UDD}$ as defined by (1) is that one gains an order in t with each pulse added [9, 15]. So no exponential costs arise.

Up to $n = 5$ the intervals of the UDD sequence were found even earlier by explict general calculation, not relying on a specific model [18]. Based on numerical evidence and on analytical evaluation of the first orders up to $n = 14$ by large-scale recursions it was subsequently conjectured that (1) applies to all pure dephasing models [15, 19]. It is not specific to the spin-boson model

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at all. Very recently, this well-founded hypothesis could be turned into a theorem by mathematical proof [20]. The caveat of this approach so far is that it can only deal with pure dephasing or longitudinal relaxation, respectively. In particular for so-called low-field systems, where the splitting between the two energy levels of the qubit is small, this is a serious drawback. In such systems, the commonly used rotating-frame approximation works only poorly and so dephasing and spin flips have to be taken into account.

So we are faced with two interesting sequences, CDD and UDD, both with strong points (CDD can eliminate all couplings, UDD requires only linear number of pulses) and weak points (CDD requires exponentially large number of pulses, UDD eliminates only pure dephasing). In the present work, we show that their combination leads to the partial combination of their advantages.

In the following derivation we will consider ideal, instantaneous π pulses for simplicity. Such pulses can be approximated to some extent by very short pulses (but see also the results in Refs. 21, 22) and, more efficiently, by suitably shaped pulses [23, 24].

To derive the advantages of a concatenated UDD sequence (CUDD) we first recall that a UDD sequence of n pulses with π rotations (Z) about the z direction suppresses the relaxation along z [20], i.e., very little spin flips occur. Formally we start from the most general decoherence Hamiltonian of a single qubit

$$H = \sum_{\gamma\in\{0,x,y,z\}} \sigma_\gamma \otimes A_\gamma, \tag{2}$$

where σ_0 is the identity in the Hilbert space of the qubit and the A_γ are operators of the environment only. Then the time evolution $p^n_{\rm UDD}$ of the UDD sequence

$$p^n_{\rm UDD} = f_{t-\tilde\delta_n} Z\, f_{\tilde\delta_n-\tilde\delta_{n-1}} Z \ldots Z\, f_{\tilde\delta_3-\tilde\delta_2} Z\, f_{\tilde\delta_2-\tilde\delta_1} Z\, f_{\tilde\delta_1} \tag{3}$$

behaves as if an effective Hamiltonian $H^{\rm eff}$ acted

$$p^n_{\rm UDD} = \exp(-itH^{\rm eff}) + \mathcal{O}(\alpha t^{n+1}) \tag{4}$$

where $\alpha := \max_\gamma(||A_\gamma||)$ is used; any operator norm $||\cdot||$ can be employed. The effective Hamiltonian $H^{\rm eff}$ only contains powers in σ_x and σ_y which are in total even, besides arbitrary powers in σ_z. Because an even power in σ_x or σ_y equals the identity and $\sigma_x\sigma_y = i\sigma_z$ we know

$$H^{\rm eff} = \sum_{\gamma\in\{0,z\}} \sigma_\gamma \otimes A^{\rm eff}_\gamma, \tag{5}$$

i.e., it only contains dephasing terms. The order of the effective bath operators obviously read

$$||A^{\rm eff}_0|| \;=\; \mathcal{O}(\max(||A_0||, t||A_x||^2, t||A_y||^2)) \tag{6a}$$
$$||A^{\rm eff}_z|| \;=\; \mathcal{O}(\max(||A_z||, t||A_x||||A_y||)). \tag{6b}$$

Note that the $A^{\rm eff}_\gamma$ are complicated, non-linear functions of t due to the control sequence.

On this level, the idea to build another DD sequence based on (5) is very appealing because it is a pure dephasing Hamiltonian. The seemingly most efficient way is to use another UDD sequence on top of (3), but now about the x- or the y-direction. Unfortunately, this is not possible since $H^{\rm eff}$ is not independent of t. Hence, if the UDD sequence requires the Hamiltonian to be applied for a given duration this cannot be done by choosing some interval t. The dependence of $H^{\rm eff}$ on t is highly non-trival because it is non-linear and because $[H^{\rm eff}(t), H^{\rm eff}(t')] \neq 0$ for $t \neq t'$.

The situation is better if one is not aiming at arbitrary intervals but at commensurate intervals $\{t_j\}$ which can be made from integer multiples of a basic interval Δt like $t_j = n_j\Delta t$ with $n_j \in \mathbb{N}$. Then one may choose $t = \Delta t$ and generate $\exp(-in_j tH^{\rm eff})$ by applying the UDD sequence n_j times. But the intervals $\tilde\delta_{j+1} - \tilde\delta_j$ are in general not commensurate, but see below. Only its most basic versions, the spin-echo for $n = 1$, and the CPMG cycle for $n = 2$ only use commensurate intervals. This is already an interesting observation since the CPMG sequence $p_{\rm CPMG}$ suppresses dephasing up to order t^3 as can be seen by regarding CPMG as the $n = 2$ case of either UDD [9] or CDD, see also below.

To assess the possible gain in concatenating CPMG with a UDD sequence $p^m_{\rm UDD}$ of m pulses and duration t_1 we estimate that the neglected term in (4) is of the order of $(\alpha t_1)^{m+1}$ This is the error committed on the UDD level of the sequence. On the next level we consider

$$p_{\rm CPMG} = p^m_{\rm UDD} X p^m_{\rm UDD} p^m_{\rm UDD} X p^m_{\rm UDD} \tag{7}$$

so that the total duration is $t = 4t_1$. Then we have $p_{\rm CPMG} = \mathbb{1} + R$ where the deviation R is estimated to be of the order of $||R|| = (\alpha^{\rm eff} t/8)^3$ with $\alpha^{\rm eff} := \max_\gamma(||A^{\rm eff}_\gamma||)$. The validity of the factor $1/8$ becomes obvious in the generalization of the CPMG to arbitrary level of concatenation below.

So the total deviation $R^{\rm tot}_{\rm CPMG-UDD}$ will be approximately

$$||R^{\rm tot}_{\rm CPMG-UDD}|| \approx \max((\alpha^{\rm eff} t/8)^3, (\alpha t/4)^{m+1}). \tag{8}$$

As expected one has to compare expressions involving different powers of t. The use of $m > 2$ is justified if $\alpha^{\rm eff}$ is much smaller than 2α. In view of (6) this will be the case if α and $\alpha^{\rm eff}$ are dominated by the $||A_\gamma||$ with $\gamma \in \{x, y, z\}$ and if $||A_z|| \ll ||A_x||$ and $||A_z|| \ll ||A_y||$. This observation shows that already a single concatenation step on top of the optimized UDD sequences can be very useful. Moreover, it is possible to pass to iterated CPMG sequences concatenated with basic UDD building blocks as in $p_{\rm iCPMG} = (p^m_{\rm UDD} X p^m_{\rm UDD})^{2c}$ with $t_1 = t/(2c)$, where c is the number of iteration cycles. Though the overvall order in the duration is not changed by the iteration the influence of the unwanted couplings which are averaged to zero becomes smaller and smaller on increasing c. This is so because the intervals between pulses

become smaller and smaller, see for instance Ref. 15 for data for the bosonic dephasing model.

If the order t^3 of the CPMG is insufficient further levels of concatenations can be added to reach higher orders. To see this it suffices to consider the simplemost building block of concatenation [17]

$$p_{n+1} = p_n X p_n X \tag{9}$$

If the time evolution p_n is governed by $H^{(n)} = \sum_{\gamma\in\{0,z\}} \sigma_\gamma \otimes A_\gamma^{(n)}$ the Magnus expansion [25] straightforwardly implies the recursion

$$\tau_n = 2\tau_{n-1} \tag{10a}$$
$$A_0^{(n+1)} = A_0^{(n)} + \mathcal{O}(\alpha_n \tau_n^2) \tag{10b}$$
$$A_z^{(n+1)} = i(\tau_n/2)[A_0^{(n)}, A_z^{(n)}] + \mathcal{O}(\alpha_n \tau_n^2) \tag{10c}$$

between consecutive levels of concatenation where τ_n is the total duration of p_n and $\alpha_n := \max_{\gamma\in\{0,z\}} ||A_\gamma^{(n)}||$.

Several remarks are in order: (i) The twofold concatenation according to (9) yields the CPMG sequence: $p_2 = p_0 X p_0^2 X p_0$ because $X^2 = \mathbb{1}$. (ii) If one starts with bath operators A_0 and A_z no terms in x- or y-direction are generated. (iii) Note that it is sufficent to consider the leading orders of the Magnus expansion to derive (10) because we are only interested in the leading deviations. (iv) The number a_n of X pulses grows roughly like 2^n. More precisely, it grows like $a_{n+1} = 2a_n + 2(-1)^n$. Starting from $a_0 = 0$ this implies the exponential law $a_n = (2/3)(2^n - (-1)^n)$.

The essential point is that in z-direction each level of concatenation introduces an additional factor of τ_n, see (10c). So each level of concatenation suppresses decoherence by an additonal order in the total duration of the pulse sequence. The pure bath operator $A_0^{(n)}$ does not affect the qubit. This kind of property was exploited in Refs. 8, 17 to establish CDD. Hence, if we concatenate n times according to (9) we will achieve a sizable suppression of decoherence due to high powers in the total duration.

More quantitatively, instead of (8) we have

$$||R_{\rm CUDD}^{\rm tot}|| \approx \max\left((\alpha^{\rm eff} t 2^{\frac{-n(n+1)}{2}})^{n+1}, (\alpha t 2^{-n})^{m+1}\right), \tag{11}$$

where t is the total duration of the entire sequence. The factor $2^{-n(n+1)/2}$ in the first term results from the product of all the τ_n obeying the recursion (10a). The factor 2^{-n} in the second term results from the number 2^n of UDD basic building blocks; each UDD interval has length $t2^{-n}$. Taking (6) into account we can conclude that $\alpha \le \alpha^{\rm eff}$ for short enough times. Then we arrive at the following conservative, but simple, estimate $||R_{\rm CUDD}^{\rm tot}|| \approx (\alpha t 2^{-m})^{m+1})$ for $n = m$. Hence we realize that the combination of concatenation and interval optimization makes it indeed possible to reduce any type of coupling to high order.

In assessing the gain of the advocated CUDD over the known CDD approach, we have to consider the number of necessary pulses. In order to make the t^m term vanish the CDD approach requires 4^m pulses [8, 17]. The CUDD (concatenated UDD) sequence on concatenation level n made from UDD sequences with m pulses requires $a_n \approx (2/3)(2^n - (-1)^n)$ pulses of type X and $m2^n$ pulses of type Z. To suppress all t^m terms we choose $n = m$ and the total number of pulses is about $(m + 2/3)2^m$. Thus we have achieved a substantial reduction by passing from 4^m to $(m+2/3)2^m$ if we replace CDD by CUDD. So one factor 2^m is reduced to the linear factor $m + 2/3$ due to the UDD building blocks. Note that this pays already for small $m \ge 1$. This is the main general result of the present work.

Unfortunately, the suppression of the dephasing component along σ_z could not be reduced in the same fashion from exponential to linear by employing UDD due to commensurability problems, see above. If one were able to use a UDD scheme also for the second step the number of pulses could be brought down to the order m^2. In practice, it can be promising to check out a work-around. The function $d(x) = \sin^2(\pi x/2)$ on the right hand side of (1) ($x = j/(n+1)$) has a simple shape, see Fig. 1. It is odd about $(1/2, 1/2)$, it vanishes at $x = 0$, and it has vanishing slope at $x = 0$ and $x = 1$. These features are reproduced by a simple third order polynomial $d_{\rm approx} = -2x^3 + 3x^2$ which approximates $d(x)$ very well as shown in Fig. 1. The maximum difference is only about 0.01 so that it is to be assumed that the use of $d_{\rm approx}(x)$ instead of $d(x)$ is hardly noticeable in practice.

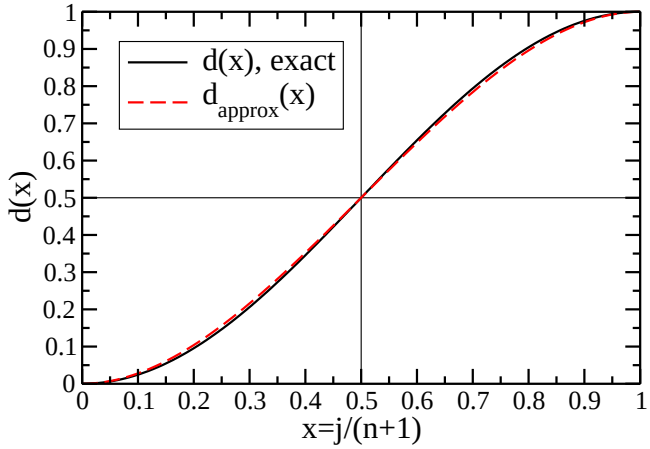

FIG. 1: (color online) Right hand side $d(x) = \sin^2(\pi x/2)$ of Eq. (1) compared to $d_{\rm approx} = -2x^3 + 3x^2$.

The use of $d_{\rm approx}(x)$ recovers commensurability. Because $x = j/(n+1)$ and the third power in $d_{\rm approx}(x)$ is the highest power occurring, all instants $\tilde{\delta}_j = d_{\rm approx}(j/(n+1))$ are integer multiples of $t/(n+1)^3$[26]. This means that we have to realize $(n+1)^3$ intervals of

UDD sequences with n Z-pulses and at the n instants $\tilde{\delta}_j$ another n X-pulses are needed. Hence this type of UDD sequence on top of a UDD sequence (approximate UDD^2) requires $n(n+1)^3+n$ pulses, hence only a polynomial law as opposed to the CUDD which still requires an exponential number of pulses. Due to the high power of the polynomial (degree 4), the approximate UDD^2 pays only for larger values of n if $(n+1)^3 \lessapprox 2^n$, i.e., for $n \gtrapprox 10$. Further exploration of the approximate UDD^2 by numerical means is called for because of the approximation involved which precludes a rigorous analytic assessment.

In summary, we have shown that UDD can be used as a powerful building block in more complex pulse sequences. Thereby the restriction of being applicable only to the suppression of either pure dephasing or pure relaxation is abolished. Three schemes are proposed. The first is suited for anisotropic situations where spin flips are much less likely than dephasing. The UDD can be inserted in a CPMG cycle. The CPMG can also be iterated if needed. This scheme yields a suppression in t^3 only due to the properties of the CPMG. But in view of the robust properties of the CPMG cycle this may be fully sufficient in many circumstances.

The second, most general and flexible, scheme consists in using the UDD sequence as starting sequence of concatenation to achieve a concatenated UDD (CUDD). This scheme makes it possible to suppress decoherence to arbitrary order t^{m+1} in the total duration t if a UDD sequence of m pulses is concatenated m times. The necessary number of pulse scales like $m2^m$ which is still exponential but considerably less demanding than 4^m as in CDD.

Third, an approximate scheme of two concatenated UDD sequences is proposed. The appoximation is needed on the second level to retrieve a certain degree of commensurability. The required number of pulses scales like m^4 so that it becomes more advantageous than CUDD for a sufficiently large number of pulses ($m \gtrapprox 10$).

The proposed schemes are expected to be experimentally useful for high-precision NMR where narrow linewidths are a prerequisite or for long-time data storage in realizations of quantum information devices.

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